

δ -CuTi ($L2_a$) Structure: AB_tP2_123_a_d-002

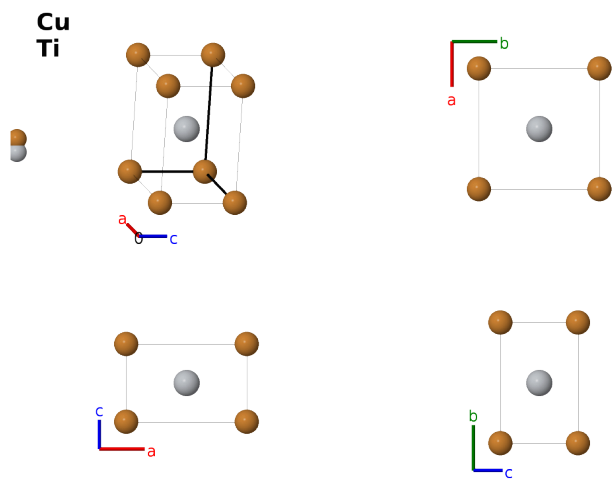
This structure previously used the label(s) **AB_tP2_123_a_d.CuTi**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/C9G2>

https://aflow.org/prototype-encyclopedia/AB_tP2_123_a_d-002



Prototype	CuTi
AFLOW prototype label	AB_tP2_123_a_d-002
<i>Strukturbericht</i> designation	$L2_a$
ICSD	103127
CCDC	1661079
Pearson symbol	tP2
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	<code>aflow --proto=AB_tP2_123_a_d-002 --params=a,c/a</code>

Other compounds with this structure

HgMn

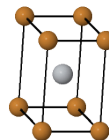
- As we have been unable to find a copy of (Karlsson, 1951), we obtained the value $a = 4.44\text{\AA}$ from (Pearson, 1958). The ICSD entry uses $a = 3.14\text{\AA}$, referencing the original publication. For now we will continue to use the value from (Pearson, 1958).

- This structure has the same AFLOW designation, AB_tP2_123_a_d, as CuAu ($L1_0$). The only difference in the structures is the c/a ratio. $L1_0$ has $c/a \approx \sqrt{2}$, characteristic of face-centered cubic ordering, while $L2_a$ has $c/a \approx 1$, a body-centered cubic-like system.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$

a1 a2 a3



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) Cu I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(1d) Ti I

References

- [1] N. Karlsson, *An X-Ray Study of the Phases in the Copper-Titanium System*, J. Inst. Met. **79**, 391–405 (1951).

Found in

- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

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